

Non-classical Role of Potential Energy in Adiabatic Quantum Annealing

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Adiabatic quantum annealing is a paradigm of analog quantum computation, where a given computational job is converted to the task of finding the global minimum of some classical potential energy function and the search for the global potential minimum is performed by employing external kinetic quantum fluctuations and subsequent slow reduction (annealing) of them. In this method, the entire potential energy landscape (PEL) may be accessed simultaneously through a delocalized wavefunction, in contrast to a classical search, where the searcher has to visit different points in the landscape (i.e., individual classical configurations) sequentially. Thus in such searches, the role of the potential energy might be significantly different in the two cases. Here we discuss this in the context of searching of a single isolated hole (potential minimum) in a golf-course type gradient free PEL. We show, that the quantum particle would be able to locate the hole faster if the hole is deeper, while the classical particle of course would have no scope to exploit the depth of the hole. We also discuss the effect of the underlying quantum phase transition on the adiabatic dynamics.

I. INTRODUCTION

Adiabatic quantum annealing (AQA) [1]-[12] is a method of finding the ground state (minimum energy state) of a given classical Hamiltonian by employing external quantum fluctuations and subsequent adiabatic reduction of them. One is given with a classical

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Hamiltonian \mathcal{H} , which may be a physical Hamiltonian with many degrees of freedom, or a suitable mathematical function depending on many variables, and the task is to determine its global minimum. In order to introduce the quantum fluctuations necessary for the AQA of such a Hamiltonian, one adds a quantum kinetic part $\mathcal{H}'(t)$ to it, such that $\mathcal{H}'(t)$ and \mathcal{H} do not commute. Initially, one keeps $|\mathcal{H}'(t=0)| \gg |\mathcal{H}|$ so that the total Hamiltonian $\mathcal{H}_{tot}(t) = \mathcal{H}'(t) + \mathcal{H}$ is well approximated by the kinetic part only ($\mathcal{H}_{tot}(0) \approx \mathcal{H}'(0)$). If the system is initially prepared to be in the ground state of $\mathcal{H}'(0)$ (one chooses $\mathcal{H}'(0)$ to have a easily realizable ground state) and $\mathcal{H}'(t)$ is reduced slowly enough, then according to the adiabatic theorem of quantum mechanics, the overlap $|\langle\psi(t)|E_-(t)\rangle|$, between the instantaneous lowest-eigenvalue state $|E_-(t)\rangle$ and the instantaneous state of $|\psi(t)\rangle$ of the evolving system, will always stay near its initial value (which is close to unity, since $\mathcal{H}_{tot}(0) \approx \mathcal{H}'(0)$). Hence at the end of such an evolution, when $\mathcal{H}'(t)$ is reduced to zero at $t = \tau$ (the annealing time), the system will be found in a state $|\psi(\tau)\rangle$ with $|\langle\psi(\tau)|E_-(\tau)\rangle| \approx 1$, where $|E_-(\tau)\rangle$ is the ground state of $\mathcal{H}_{tot}(\tau)$, which is nothing but the surviving classical part \mathcal{H} . Thus at the end of an adiabatic annealing the system is found in the ground state of the classical Hamiltonian with a high probability. Based on this principle, algorithms can be framed to anneal complex physical systems like spin glasses as well as the objective functions of hard combinatorial optimization problems (like the Traveling Salesman Problem), towards their ground (optimal) states [2, 6, 8, 11].

In order to ensure adiabaticity, the evolution should be such that

$$\tau \gg \alpha; \quad \alpha = \frac{|\langle\dot{\mathcal{H}}_{tot}\rangle|_{max}}{\Delta_{min}^2}, \quad (1)$$

where

$$\begin{aligned} |\langle\dot{\mathcal{H}}_{tot}\rangle|_{max} &= \max_{0 \leq s \leq 1} \left[\left| \left\langle E_-(s) \left| \frac{d\mathcal{H}_{tot}}{ds} \right| E_+(s) \right\rangle \right| \right] \\ \Delta_{min}^2 &= \min_{0 \leq s \leq 1} [\Delta^2(s)]; \quad s = t/\tau; \quad 0 \leq s \leq 1, \end{aligned} \quad (2)$$

$|E_+(t)\rangle$ being the instantaneous first excited state of the total Hamiltonian $\mathcal{H}_{tot}(t)$, $\Delta(t)$ being the instantaneous gap between the ground state and the first excited state energies and α being the adiabatic factor (for a simple proof see [14]).

One key feature, believed to be behind the success of AQA over the classical ones [2, 6, 8] in glass-like rugged PEL, is the ability of the quantum systems to tunnel easily through potential energy barriers even if they are very high, provided they are narrow enough, in

contrast to the the classical ones, which always has to scale the barrier height with its kinetic energy (temperature) irrespective of the width [5, 7, 10, 13, 15]. Here we show that there is another aspect which makes a quantum mechanical searcher more advantageous over the classical ones- it can utilize the depth of the potential energy minimum in locating it in absence of any potential gradient which a classical searcher cannot.

II. SEARCHING A HOLE ON A GRADIENT-FREE PEL

We consider a lattice with N sites, $|i\rangle$ denoting the state of a particle localized at the i -th site. At each site, there is a potential, which is zero at all the sites $i \neq w$, and is $-\chi$ at $i = w$, where w is chosen randomly. Thus the PEL is essentially a flat one without any gradient, with a single hole (minimum) at $i = w$ with a depth χ . This is precisely some kind of analog version of Grover's algorithm for searching a particular entry in an unstructured database [16] - [18]. But in those studies, the possibility of utilizing the depth of the hole in favor of faster search was not considered, and the gain over the classical ones is limited by the optimal Grover's bound of $\mathcal{O}(\sqrt{N})$ speed-up [18, 19].

Let us consider that the lattice points are connected to each other by an infinite range hopping term Γ between any two sites. The question is how fast a particle can locate the hole starting from a state which does not assume any knowledge of the position of the hole, by reducing its kinetic energy Γ , and tuning the hole depth χ . The Hamiltonian for a particle on such a lattice will be given by-

$$\mathcal{H}_{tot}(t) = -\chi(t)|w\rangle\langle w| - \Gamma(t) \sum_{i,j;i \neq j} |i\rangle\langle j|; \quad \chi(t), \Gamma(t) > 0. \quad (3)$$

In order to anneal the particle to the hole, one has to reduce Γ from a very high value to a very low final value and tune χ in the opposite manner, so that $\Gamma(t = 0) \gg \chi(t = 0)$ and $\Gamma(t = \tau) \ll \chi(t = \tau)$, where τ is the annealing time. The evolution should satisfy the adiabatic condition (1). The eigen-spectrum of $\mathcal{H}_{tot}(t)$ consists of a ground state $|E_-(t)\rangle$ and first excited state $|E_+(t)\rangle$ (in the order of increasing eigen values) with energies

$$E_{\pm}(t) = -\frac{1}{2} \left[(N-2)\Gamma + \chi \pm \sqrt{(N\Gamma - \chi)^2 + 4\chi\Gamma} \right] \quad (4)$$

respectively, all the time dependencies being implicit, through the time dependence of Γ and

χ . The instantaneous gap is thus given by

$$\Delta(t) = \left| \sqrt{(N\Gamma - \chi)^2 + 4\chi\Gamma} \right|. \quad (5)$$

The instantaneous first and second excited states $|E_{\pm}(t)\rangle$ are given by -

$$|E_{\pm}(t)\rangle = \frac{1}{\sqrt{C_{\pm}^2(t) + N - 1}} \left[C_{\pm}(t)|w\rangle + \sum_{i \neq w}^N |i\rangle \right], \quad (6)$$

where

$$C_{\pm}(t) = \frac{1}{2\Gamma} [-(N - 2)\Gamma + \chi \mp \Delta] \quad (7)$$

The second excited state is $(N - 2)$ -fold degenerate, with eigenvalue $-\Gamma$, and the time evolving Hamiltonian never mixes the first two eigenstate with any of the second excited states. This can be easily argued noting that a state of the form $|E_2\rangle = \frac{1}{\sqrt{2}}(|i\rangle - |j\rangle)$ ($i, j \neq w$) is an eigenstate of $\mathcal{H}_{tot}(t)$ with eigenvalue $-\Gamma$, and $\langle E_2|E_{-}(t)\rangle = \langle E_2|E_{+}(t)\rangle = 0$ for all t . For all allowed combinations of i and j we get $(N - 2)$ such linearly-independent eigenstates. Form these $(N - 2)$ linearly-independent eigenstates we can construct $(N - 2)$ mutually orthogonal eigenstates, each of which will obviously satisfy the above non-mixing condition. Thus we have to take care of only two lowest lying states and the gap between them. Henceforth we will consider only the large N limits, and replace ' $=$ ' by ' \approx ' when the correction will vanish in the said limit.

In investigating the condition of adiabatic evolution we consider two separate cases. In general, in a quantum annealing program, one might not have the facility of tuning both the potential energy part and the kinetic part in practice, since, say, one might depend on the strength of interactions between the elementary constituents (hard to tune), while the other might be introduced through an applied external field (easily tunable). Hence in our analysis we have considered two separate cases - in the first case we tune χ keeping Γ constant, while in the second case we do the reverse.

A. Constant- Γ Annealing

We start with the initial state $|\psi(0)\rangle = \frac{1}{\sqrt{N}} \sum_i^N |i\rangle$ (which is of course the ground state of $\mathcal{H}_{tot}(0)$) and adopt a linear annealing schedule:

$$\Gamma = \Gamma_0; \quad \chi = \chi_0 \frac{t}{\tau}; \quad \chi_0 = rN\Gamma_0. \quad (8)$$

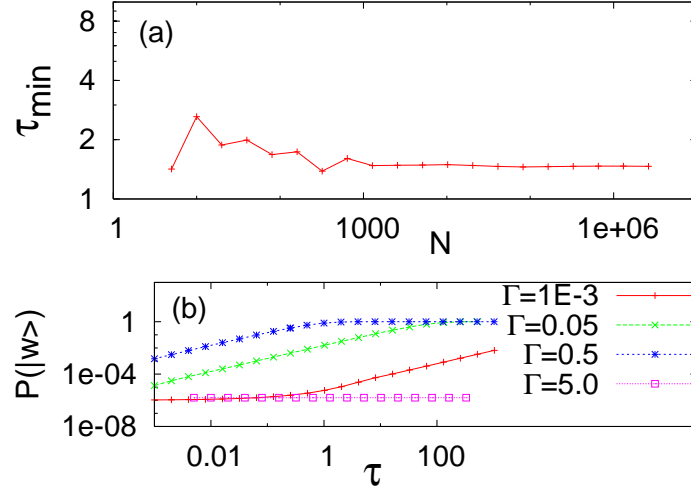


FIG. 1: Panel (a) in the figure shows the variation of the minimum time τ_{min} required to achieve the target success probability $P_T = 0.33$ for the constant- Γ annealing ($\Gamma(t) = \Gamma_0$, $\chi(t) = \chi t/\tau$; $r = 2.0$, $\Gamma_0 = 0.5$), obtained by solving the time-dependent Schrödinger equation numerically. Panel (b) shows the variation of final probability $P(|w\rangle)$ of finding the system in state $|w\rangle$, with annealing time τ , for different final value of Γ . Here we have taken $N = 10^6$.

Here r is an arbitrary factor which might also depend on N . When Γ is kept constant, we have to keep it sufficiently low (or, in other words, χ_0 sufficiently high), so that the ground state of $\mathcal{H}_{tot}(\tau)$ has a substantial (non-vanishing in the $N \rightarrow \infty$ limit) overlap with $|w\rangle$. At $t = \tau$, we get from Eq. (7), the amplitude of $|w\rangle$ in the final ground state to be $C_-(\tau)/\sqrt{C_-^2(\tau) + N - 1}$, where

$$C_-(\tau) = 1 + \frac{N(r-1)}{2} + \frac{\left| \sqrt{N^2(r-1)^2 + 4rN} \right|}{2}. \quad (9)$$

Clearly, if $r > 1$, then the amplitude $C_-(\tau) \gtrsim N$, and thus the overlap amplitude $\sim \mathcal{O}(1)$, whereas if $r < 1$, then $C_-(\tau) \sim 1$, and the amplitude vanishes as $N \rightarrow \infty$. Thus to be able to locate the hole at the end, we have to take $r > 1$. In fact, The adiabatic factor in that case ($r > 1$) is given by

$$\alpha_1 = \frac{|\langle \dot{\mathcal{H}}_{tot}(t) \rangle|_{max}}{|\Delta^2(t)|_{min}} = \left(\frac{r\Gamma_0^2}{\tau} \right) \frac{N\sqrt{N-1}}{|\Delta^3(t)|_{min}} \quad (10)$$

This has its maximum at $t_m = \tau(N-2)\Gamma_0/\chi_0 \approx \tau/r$, and the maximum value is given by

$$\alpha_1 = \frac{\chi\sqrt{N}}{8\Gamma_0^2(N-2)^{3/2}} \approx \frac{r}{8\Gamma_0}. \quad (11)$$

This clearly shows that if the hole-depth χ_0 scales linearly with the size N of the search space (i.e., r is independent of N), the search can be completed in a time independent of N . We calculated numerically the minimum time τ_{min} required for obtaining a targeted success probability $P_T = |\langle \psi(\tau) | w \rangle|^2 = 0.33$ for different N , through many decades. The evolution is computed solving time-dependent Schrödinger equation numerically and τ_{min} is figured out up to an accuracy of 10^{-4} employing the following bisection scheme. We first figure out arbitrarily a high value of τ (call it τ_{hi}) for which $P(|w\rangle) \equiv |\langle \psi(\tau) | w \rangle|^2 > P_T$. Next we find a low τ (τ_{lo}), for which $P(|w\rangle) < P_T$. Then we evaluate $P(|w\rangle)$ for $\tau = \tau_m = (\tau_{hi} + \tau_{lo})/2$. If the result is greater than P_T , then we replace τ_{hi} by τ_m (and retain old τ_{lo}), else we replace τ_{lo} by τ_m (and retain old τ_{hi}) and repeat the same process. We go on iterating until the value of $|P(|w\rangle) - P_T|$ for both τ_{hi} and τ_{lo} lies within some desired accuracy limit. The results (Fig. 1a) clearly show that $P(|w\rangle)$ becomes independent of N for large N , as expected.

The relaxation behavior for large N for a given annealing time τ of course depends on the value of Γ_0 (see Fig. 1b). If Γ_0 is too small, the system takes a longer time to feel the changes in the landscape, and hence the adiabatic relaxation requires longer time (the adiabatic factor becomes bigger; see Eq. 11). On the other hand, if Γ_0 is too large, the ground state itself is pretty delocalized, and hence the final state, though more closer to the ground state, has again a small overlap with the target state $|w\rangle$. For $\Gamma_0 \approx 0.5$, the schedule is found to be optimal (Fig. 1(b)). The relaxation behavior is seen to be linear with the annealing time τ for large τ .

B. Constant- χ Annealing

Next, we consider the case where χ is kept fixed and Γ is reduced linearly, i.e., $\chi = \chi_0 = rN\Gamma_0$ and $\Gamma = \Gamma_0(1 - t/\tau)$. In this case, we start with the same democratic initial state $|\psi_0\rangle$ as in the previous case, which is not of course the ground state in presence of the hole (we cannot construct the actual initial ground state without the explicit knowledge of the location of the hole). All we need to show in this case, is that it has a non-vanishing (i.e., non-zero in the $N \rightarrow \infty$ limit) overlap $|\langle \psi(0) | E_-(0) \rangle|$ between our initial state and the true ground state at $t = 0$. If we can assure adiabaticity for the subsequent evolution, this overlap will be conserved and would emerge as the final overlap between $|\psi(\tau)\rangle$ and $|w\rangle$. Calculation similar to that of the previous section shows that, for $r < 1$, $C_-(0) \rightarrow 0$ as

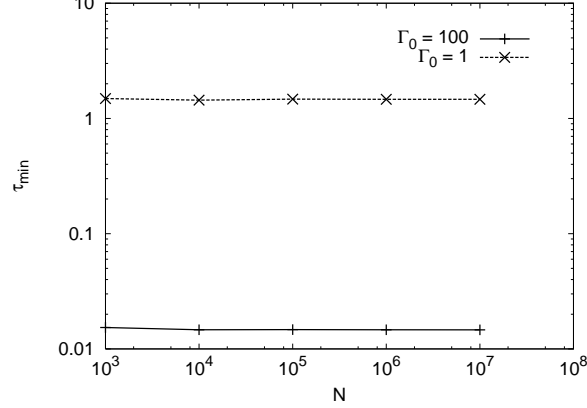


FIG. 2: The figure shows variation of the minimum time τ_{min} required to achieve success probability $P_T = 0.9$, with N for the constant- χ annealing. The result is obtained by solving the time-dependent Schrödinger equation numerically with $\Gamma(t) = \Gamma_0(1 - t/\tau)$, $\chi(t) = \chi_0 = r\Gamma_0 N$ for $r = 0.5$.

$N \rightarrow \infty$, implying that the overlap actually tends to unity in that limit, while it vanishes for $r > 1$. The adiabatic factor in the former case ($r < 1$) is given by

$$\alpha_2 \approx \frac{1}{8\Gamma_0 r^2}, \quad (12)$$

which is again a constant independent of N , if r is N -independent (i.e., χ_0 is linear in N). We present a similar numerical calculation, as in the previous section, for the variation of τ_{min} with N in Fig. (2). It shows that the value of τ_{min} becomes independent of N in the large- N limit (its asymptotic value, however depends on Γ_0).

III. THE UNDERLYING TRANSITION

Let us concentrate on the rather interesting case of N -independent r . The expression for the gap Δ (Eq. 5) shows that the gap scales linearly with N everywhere except at the point $N\Gamma = \Gamma_c = \chi$, where it scales as \sqrt{N} . In our notation, this happens at the instant $t^* = \tau/r$ in the case of constant- Γ annealing, and at $t^{**} = \tau(1 - r)$ in the constant- χ case. For successful annealing one cannot avoid this point during the evolution in both cases. To see what happens at that point, let us focus on the amplitude $|\langle w|E_-(\chi, \Gamma)\rangle|$ for $\Gamma > \Gamma_c$ and $\Gamma < \Gamma_c$. Let us consider, say, the Γ -constant annealing case. We have from Eq. (7), $C_-(t) \approx (-N\Gamma_0(1 - rt/\tau) + N\Gamma_0|1 - rt/\tau|)/2\Gamma_0$. Taking the modulus into account, one finds $C_-(t) \approx 0$ for $t < t^*$ (which means the amplitude vanishes), while $C_-(t) \sim N$ for $t > t^*$ (the

amplitude tends to unity). This means the ground state of $\mathcal{H}_{tot}(\chi, \Gamma)$ undergoes a global change in character from a completely delocalized one to a completely localized one at this special point. Thus, to follow the ground state, a lot of tunneling from all the sites to the hole is required at the point. Here the depth of the hole plays a crucial role in making this tunneling possible preventing the gap Δ from closing at the transition point. If however, the system passes this point very fast, this massive tunneling might remain incomplete and a resultant loss in the adiabaticity may occur. Similar argument holds for the χ -constant annealing.

If instead of the Hamiltonian we considered, one takes a bounded version of it (energy not growing with N), say, by keeping χ independent of N and scaling Γ_0 by N , then one can easily see that this special transition point would behave like a true quantum critical point with the gap vanishing as $1/\sqrt{N}$ [17]. The two states- the one localized at the hole and the other delocalized over the entire lattice, have exactly equal energies at this “critical” point as the gap closes. But before reaching that point (i.e., in the kinetic energy dominated region), the ground state is non-degenerate and delocalized, while after the point (i.e., in the potential energy dominated region) the ground state is degenerate and localized at the hole. Since there is no energy difference between the two states (the localized and the delocalized ones) at the critical point, the evolving system cannot sense the global exchange of character between the ground state and the first excited state at this point and thus fails to adopt (tunnel) accordingly to follow the ground state. Letting the hole scale linearly with N and taking infinite range hopping, one prevents the gap from closing, and thus favors the localized state energetically over the delocalized one at the transition point. This acts as a drive for the necessary tunneling and thus provides a guidance for the system to follow the ground state as it changes its global character.

However, it is also worth noting that increasing the hole-depth χ_0 indiscriminately does not pay. In the case of constant- Γ annealing, the adiabatic factor increases with r (Eq.11), which means we have to keep r as small as possible, i.e., $r \rightarrow 1$ gives the best result. This can be explained by noting that a larger χ_0 would demand a slower rate of evolution if adiabaticity is to be ensured. In the constant- χ case, adiabatic factor decreases with r , but one has to keep $r < 1$, which means χ can be increased only linearly with N , up to the upper limit $N\Gamma_0$ in order to accelerate the annealing effectively. This is because, too big χ_0 implies too much error in the initial state and the overlap is negligible right from the onset.

Hence even with a perfectly adiabatic evolution we end up with the negligible overlap.

To summarize, we studied the adiabatic searching of a gradient-free potential energy landscape on a lattice with a randomly placed single isolated minimum (hole) by a quantum searcher. We have found that the depth of the hole plays a non-classical role in accelerating the search. This is because the delocalized wave-function of the quantum adiabatic searcher can detect the hole from the very onset of the search and keep track of it, in contrast to a classical searcher, who of course cannot sense the hole depth non-locally and utilize it. We found that the condition for adiabatic search requires an infinite-range hopping between the points in the PEL and the depth of the hole to scale linearly with the lattice-size N . We have discussed how the hole-depth plays a role in preventing the closure of the gap and the consequent divergence of the searching time.

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